

1,3-Dichlorobenzene  
541-73-1 | DTXSID6022056

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.43 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.94e-01

Confidence level: 8.81e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Thiazole, 2,4-dimethyl-</div> <div>Measured: 2.15</div> <div>Predicted: 8.92</div>	<div>Image not found</div> <div>p-Cresol</div> <div>Measured: 1.74</div> <div>Predicted: 9.59e-02</div>	<div>Image not found</div> <div>Diisopropylamine</div> <div>Measured: 3.68</div> <div>Predicted: 64.3</div>
<div>Image not found</div> <div>para-Xylene</div> <div>Measured: 2.69</div> <div>Predicted: 8.88</div>	<div>Image not found</div> <div>Propylene carbonate</div> <div>Measured: 8.29</div> <div>Predicted: 5.02e-02</div>	